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Perturbative expansion of the energy eigenvalues for the planar quantum rotor based on the calculation of a finite degree secular polynomial

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Abstract

The free planar rotor system is introduced and the interaction of this system with an external electric field is studied. The quantum problem is governed by an equation of Mathieu type. This is done by evaluating a finite secular polynomial corresponding to a matrix representation of the Hamiltonian for the system. It is shown that perturbative expansions for the energy can be evaluated in powers of the coupling constant.

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From the theoretical point of view, the plane rotor has many analogies with non-Abelian gauge theories. Its unusual topology implies that the rotor system must possess different quantum realizations, which in turn implies the existence of θ-vacuum phenomena. In fact, the planar rotor presents many analogies with non-Abelian gauge theories. The rotor may allow the appearance of instantons given that the interaction term has the appropriate structure. In the path integral formalism, it arises from the contribution of closed trajectories with nonzero winding number. Given that different quantum Hamiltonians can correspond to the same classical dynamics, these θ-vacuum phenomena can also be accounted for in the Hamiltonian context in this sense [1,2]. From the physical point of view,

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the motion of electrons in a circular SQUID can be studied by means of this system [3]. In fact, experiments have been done recently on systems with such a geometry. Here, we would like to investigate the free rotor quantum problem and the planar rotor which interacts with an external electric field [4, 5]. The free rotor quantum problem has been studied from both the Hamiltonian and path integral perspectives and a description of the spectrum has been obtained corresponding to each θ-vacuum realization [5]. Some new features which seem to have gone undetected in previous work will be presented here. The quantum version of the problem is determined by a type of Mathieu equation [6]. The former problem can be solved exactly, whereas the free rotor problem interacting with an external field has to be studied in some approximation. We show that a finite secular polynomial, which is a function of the coupling constant in the Hamiltonian, can be calculated. This finite polynomial is obtained from a submatrix of the infinite Hamiltonian matrix which is constructed from the matrix elements of the Hamiltonian operator acting on a given basis set. Even though this entire matrix is an infinite matrix, finite size submatrices can be selected which can be used to calculate a finite secular polynomial. The exact number of terms depends on the order in the coupling which is desired. Although an infinite number of elements in the full exact infinite matrix are neglected in this approach, as long as the coupling is small, we are simply neglecting higher order terms in the secular polynomial. Thus, the secular polynomial depends on the coupling constant which appears in the potential term in the Hamiltonian. The matrix elements can be evaluated with respect to a particular basis; in fact, the eigenfunctions of the free rotor problem can be used. Of course, these polynomials can be used for calculation of the energies by solving for the roots of the polynomial directly as a function of the coupling constant.

This approach has also been used for finite Hamiltonian matrices in a different context [7,8]. It has been shown in [7] how to construct secular polynomials which correspond, or are equivalent to, a set of Hamiltonian matrices for various states of a particular molecular system. The technique provides a procedure for producing an essentially exact reconstruction of a given Hamiltonian matrix. A technique for interpolating between the strongly and weakly correlated cases in which the input information consists of perturbative expansions for large and small coupling is used. The idea here is to turn this method around and use an approximate secular polynomial obtained from a finite version of the actual infinite Hamiltonian matrix to generate a perturbative expansion which is valid for small values of the coupling parameter. The interesting feature of this procedure is that when the equations for the unknown coefficients are obtained, they are found in some instances to have multiple roots. Hence the series bifurcates at given orders of the coupling. This is an interesting result on its own. At the moment, we have no analytic derivation of this; however it may be conjectured that this result persists to arbitrarily high orders in the coupling giving an arbitrarily large number of such series for the energy. The technique used here is not complete or comprehensive; an exact analytic procedure would surpass what is done here.

The system which is considered here consists of a free nonrelativistic particle constrained to move on the circumference of the unit circle S^1. With the mass set equal to unity, the classical Lagrangian is given by

$$L = \frac{1}{2}\dot{\vartheta}^2, \tag{1}$$

where ϑ is the angle of the particle over the circle, where the variable $\vartheta(t)$ is restricted to the range $0 \le \vartheta \le 2\pi$.

The corresponding quantum system is defined by the related Hamiltonian

$$H_0 = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\vartheta^2}. \tag{2}$$

Since the boundary conditions are periodic, the corresponding self-adjoint extension of H is

$$D(H_0) = \{f : S^1 \to C,\ f \in AC,\ f(0) = f(2\pi)\}. \tag{3}$$

Here, AC represents absolutely continuous functions on $[0, 2\pi]$. The classical equation of motion which derives from (1) can be generated by a different Lagrangian,

$$L(\epsilon) = \frac{1}{2}(\dot{\vartheta}^2 + \epsilon)^2 - \frac{1}{2}\epsilon^2. \tag{4}$$

This gives rise to a related quantum Hamiltonian of the form

$$H(\epsilon) = -\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}\vartheta} - \mathrm{i}\epsilon\right)^2. \tag{5}$$

In the domain of (3), however, $H(\epsilon)$ has a different spectrum than H_0 if ϵ is not an integer, and thus an inequivalent quantum realization.

By imposing quasi-periodic boundary conditions, the quantum system described by (5) can be reproduced from (2). If we let H_0^ϵ be the self-adjoint extension of the operator (2) defined in the new domain

$$D(H_0^\epsilon) = \{f : S^1 \to C : f \in AC,\ f(0) = \mathrm{e}^{-2\pi \mathrm{i}\epsilon} f(2\pi)\}, \tag{6}$$

then the unitary operator, $T : L^2(S^1) \to L^2(S^1)$ defined by $T\psi(\vartheta) = \mathrm{e}^{-\mathrm{i}\epsilon\vartheta}\psi(\vartheta)$ satisfies $T^{-1}H_0^\epsilon T = H(\epsilon)$. The operators $H(\epsilon)$ and H_0^ϵ describe equivalent physical systems. The dynamics can be parametrized in terms of $\epsilon \in [0, 1)$ since H_0^ϵ and $H_0^{\epsilon+n}$ with n an integer are the same operators. Finally, as far as these operators are concerned, the solution of the spectral problem corresponding to the given Hamiltonian is required. For the operator $H(\epsilon)$, the eigenstates and eigenvalues are given by

$$\varphi_n = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}n\vartheta}, \qquad E_n^\epsilon = \frac{1}{2}(n-\epsilon)^2, \tag{7}$$

where $n = 0, \pm 1, \pm 2, \ldots$. The expression for E_n^ϵ shows that the eigenvalues of $H(\epsilon)$ and $H(\epsilon + n)$ are the same when n is an integer. The eigenstates and eigenvalues of H_0^ϵ in $D(H_0^\epsilon)$ are given by

$$\varphi_n^\epsilon(\vartheta) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}(n-\epsilon)\vartheta}, \qquad \tilde{E}_n^\epsilon = \frac{1}{2}(n-\epsilon)^2, \tag{8}$$

where $n = 0, \pm 1, \pm 2, \ldots$. These two operators are equivalent since $\tilde{E}_n^\epsilon = E_n^\epsilon$ and $\varphi_n^\epsilon(\vartheta) = T\varphi_n(\vartheta)$.

Consider the planar rotor interacting with an external electric field with the Hamiltonian

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\vartheta^2} + \lambda\cos\vartheta, \tag{9}$$

under periodic boundary conditions. A novel way of developing perturbative expansions for the eigenvalues of the corresponding eigenvalue problem will be presented. This method will produce series expansions for the energy eigenvalues which will be valid in the small λ regime. These expansions give the unperturbed form for the energy, namely $E_n = n^2/2$, when λ is set equal to zero. The idea is to calculate a finite matrix corresponding to H with respect to an arbitrary but complete set of basis functions. A secular polynomial can then be calculated corresponding to a finite submatrix formed from this infinite matrix using symbolic manipulation. The set of eigenvectors which are selected will be the eigenvectors of the free problem defined by the Hamiltonian in (2) which take the form

$$\psi_n(\vartheta) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}n\vartheta}. \tag{10}$$

A matrix representation of H can then be constructed using the functions ψ_n by evaluating the matrix elements

$$H_{ij} = \int \psi_i^* H \psi_j \, \mathrm{d}\vartheta, \qquad i, j = 1, 2, 3, \dots. \tag{11}$$

The secular matrix is generated by calculating the matrix $[H_{ij} - E\delta_{ij}]$, and the determinant of this matrix generates the characteristic polynomial by means of $\det(H_{ij} - E\delta_{ij}) = 0$. The finite secular submatrix which is used for the calculation of the polynomial will be indexed by letting i, j run between the values $-(N-1)/2, \dots, -1, 0, 1, \dots, (N-1)/2$. To evaluate the matrix elements (11) with respect to the basis (10), we evaluate the following integral:

$$\begin{aligned} H_{nm} &= \frac{1}{2\pi} \int_0^{2\pi} \mathrm{e}^{-\mathrm{i}n\vartheta} \left(-\frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}\vartheta^2} + \lambda \cos\vartheta \right) \mathrm{e}^{\mathrm{i}m\vartheta} \, \mathrm{d}\vartheta \\ &= \frac{1}{2\pi} \int_0^{2\pi} \left(\frac{m^2}{2} \mathrm{e}^{\mathrm{i}(m-n)\vartheta} + \lambda \mathrm{e}^{\mathrm{i}(m-n)\vartheta} \cos\vartheta \right) \mathrm{d}\vartheta = \frac{m^2}{2} \delta_{nm} + \frac{\lambda}{2} (\delta_{n,m+1} + \delta_{n,m-1}). \end{aligned} \tag{12}$$

For a given N, a secular polynomial can be calculated by evaluating the determinant of the submatrix $(H - EI)_{nm}$, where I is the identity matrix. From this polynomial, perturbation expansions for the energy in powers of λ can be evaluated. To do this, a series of the form

$$E = \sum_{m=0}^{\infty} c_m \lambda^m, \tag{13}$$

but truncated after a finite number of terms, is substituted into the characteristic polynomial. Expanding this out in powers of λ, the coefficients of each power of λ will yield equations which can be used to evaluate the unknown coefficients c_m which appear in the energy series (13). All of the expansions determined here are expansions about λ equal to zero.

A large polynomial can be calculated by using symbolic manipulation, and when (13) is substituted, the coefficient of λ^0 is found to be a large polynomial in c_0. Solving the polynomial for its roots, we obtain the following sequence of values:

$$c_0 = 0, \frac{1}{2}, 2, \frac{9}{2}, 8, \frac{25}{2}, 18, \dots.$$

These are precisely the unperturbed eigenvalues $E_n = n^2/2$ for $n = 0, \pm 1, \pm 2, \dots$ given above. Solutions to (13) corresponding to the first four of these eigenvalues will be developed next, using a particular value of c_0 to initialize the series. As the equations are solved out to a given order in λ, it is found that all coefficients of the odd powers of λ vanish to the order calculated. It is found that the calculated coefficients are stable under the increase of size of the submatrix. All of the series which are obtained in this way are even functions of λ. Moreover, another interesting property of these series is also obtained, which might not be apparent in another method. If we initialize the series with $c_0 = 1/2$, the equation which determines c_2 is found to be a quadratic in c_2. Thus, there are at least two distinct solutions based on this value of c_0 which separate from each other at higher order in the coupling. A graph which shows this behavior of the energy is given in Fig. 1. The same property is observed to occur

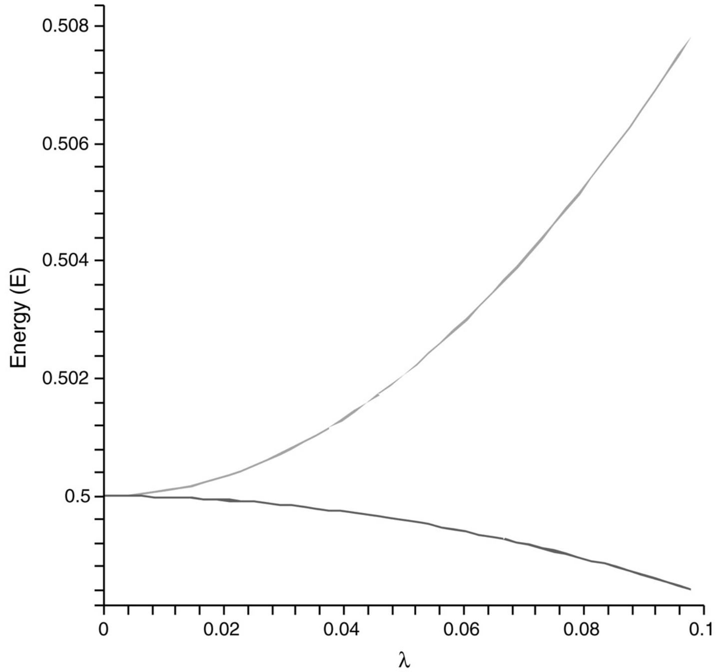

Fig. 1. Plot of the energy as a function of λ for the two series (13) which bifurcate away from $c_0 = 1/2$.

in the additional series initialized with $c_0 = 2$ and $c_0 = 9/2$, but the quadratic factors appear further on at higher order in the series. For the value $c_0 = 2$ this happens at order λ^4 and at order λ^6 for the next value $c_0 = 9/2$. It is not excluded that further bifurcations may take place at even higher orders in λ although no analytic proof is known at the moment. The first few coefficients for the perturbative series corresponding to the first four values of c_0 are presented in Tables 1 and 2. It is not hard to carry this further to even higher orders by constructing a larger matrix H and including more terms in the series (13). The radius of convergence of a series of the form (13) can be found by using the definition

$$r = \frac{1}{\limsup_{m\to\infty} \sqrt[m]{c_m}}. \tag{14}$$

For the series in Table 1, the coefficients can be used to estimate r given by (14) for any finite n, and then further asymptotic analysis can be used to produce a more precise estimate. For the series in Table 1, the following three estimates are obtained for the radius of convergence r for the series recorded there: 0.38, 1.59 and 0.38, respectively.

To conclude, these results have an immediate application to the physical problems alluded to at the start. In the free case, $\lambda = 0$ for $\epsilon = 1/2$, the ground state is seen to be degenerate, with a discontinuity in the energy's first derivative with respect to ϵ. As the interaction is applied, this degeneracy goes away for any value of λ and the separation in the $\epsilon = 1/2$ location between the first two levels grows monotonically with λ.

Table 1
Coefficients for the perturbative energy series in (13) for $c_0 = 0$ and $c_0 = 1/2$

c_0	0	$\frac{1}{2}$	$\frac{1}{2}$
c_2	-1	$-\frac{1}{6}$	$\frac{5}{6}$
c_4	$\frac{7}{4}$	$\frac{5}{432}$	$-\frac{763}{432}$
c_6	$-\frac{58}{9}$	$-\frac{289}{155520}$	$\frac{1002401}{155520}$
c_8	$\frac{68687}{2304}$	$\frac{21391}{55987200}$	$-\frac{1669068401}{55987200}$
c_{10}	$-\frac{123707}{800}$	$-\frac{2499767}{28217548800}$	$\frac{4363384401463}{28217548800}$
c_{12}	$\frac{8022167579}{9331200}$	$\frac{1046070973}{47405481984000}$	$-\frac{40755179450909507}{47405481984000}$
c_{14}	$-\frac{286241141477}{57153600}$	$-\frac{196784996207}{34131947028480000}$	$\frac{170942293775248009327}{34131947028480000}$

All coefficients with odd index are found to vanish.

Table 2
Coefficients for the perturbative energy series in (13) for $c_0 = 2$ and $c_0 = 9/2$

c_0	2	2	$\frac{9}{2}$	$\frac{9}{2}$
c_2	$\frac{1}{15}$	$\frac{1}{15}$	$\frac{1}{35}$	$\frac{1}{35}$
c_4	$-\frac{317}{27000}$	$\frac{433}{27000}$	$\frac{187}{1372000}$	$\frac{187}{1372000}$
c_6	$\frac{10049}{5315625}$	$-\frac{5701}{5315625}$	$-\frac{5861633}{181515600000}$	$\frac{6743617}{181515600000}$
c_8	$-\frac{93824197}{244944000000}$	$-\frac{112236997}{244944000000}$	$\frac{2825925629}{2846164608000000}$	$-\frac{2337184771}{2846164608000000}$
c_{10}	$\frac{21359366443}{241116750000000}$	$\frac{8417126443}{241116750000000}$	$\frac{45361065433}{1217525971200000000}$	$\frac{107856094183}{1217525971200000000}$

All coefficients with odd index are found to vanish.

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